
# HF and DFT

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# Today we will learn..

- Interaction between molcas modules
- How to run RHF and UHF calculations
- How to run DFT calculations


# Communication between codes

```
&GATEWAY
 ...
&SEWARD;  &SCF
```

- How do they communicate?
- Where are the files?

# Communication between codes

- GATEWAY
  - create new RUNFILE
  - pass returncode
- SEWARD
  - compute integrals
  - create GssOrb file
  - update RUNFILE
  - pass returncode
- SCF
  - check RUNFILE for starting orbitals
  - check ScfOrb (from another SCF run) or GssOrb file
  - compute WF, and create ScfOrb file
  - update RUNFILE

# WorkDir

How to set WorkDir?

- Special case: not set
  WorkDir – /tmp/water.$RANDOM
- WorkDir=/scratch/molcas/water/
- MOLCAS_WORKDIR=/scratch/molcas/
  the actual WorkDir name constructed as:
  MOLCAS_WorkDir + the name of Project (input filename).

# use of WorkDir

Should one reuse WorkDir?

- Yes, if want to reuse data, e.g. starting orbitals
- No, if a new calculation is too different

To run calculation with new Workdir

- rm -fr $Workdir
- MOLCAS_NEW_WORKDIR=YES
- *molcas -new input*

# Keywords for SCF

- Select configuration
  - by hands: Occupide = 3 1 1 0
  - use aufbau: Charge = 0
- Initial guess
  - Guess Orbitals
- Integrals
  - Conventional/Cholesky
  - Direct, SemiDirect
- Convergence acceleration
  - Dumping
  - C1-DIIS, C2-DIIS

# if SCF does NOT converge

- Remember: HF is a singe configuration method
- Ask yourself why do you need it?! for RASSCF?
- Try NOT to use Aufbau
- Try to remove acceleration: NoDamp, NoDIIS
- Reduce basis set, and use EXPBAS later
- Make starting orbitals for cation
- Tighten Cholesky Threshold
- Check Thresholds for convergence
- Always check that aufbau converged,
  and you have correct configuration

# keywords for UHF

- UHF
- configuration
  - Occupied = 0 1; 1 0
  - Zspin = 2 (difference between alpha and beta)
- Convergence is poorer comparing to RHF
- UHF produces two orbital files: UhfOrb and UnaOrb

# H2 molecule

```
&GATEWAY
coord = H2.xyz
&SEWARD
&SCF
UHF
```

This input contains two mistakes..

# H2 molecule

- by default $D_{2h}$ group will be selected
- you need to introduce some noise by orbital rotation

```
&GATEWAY
coord = H2.xyz
group = C1
&SEWARD
&SCF
UHF
SCRAMBLE = 0.2
```

# DFT

- DFT is computed with the same SCF module
- KSDFT=Functional
- use 'molcas help scf ksdft' to get a list

Notes.

- DFT converges slower than HF:
  smaller gap leads to 'mixing' of configurations
- Consider to use HF orbitals as starting point
- Use relatively small basis sets
- Remember that accurate grids are VERY expensive
- *MOLCAS is not the best code for DFT!*
- DFT motto: good results for unknown reasons